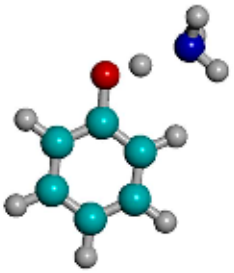

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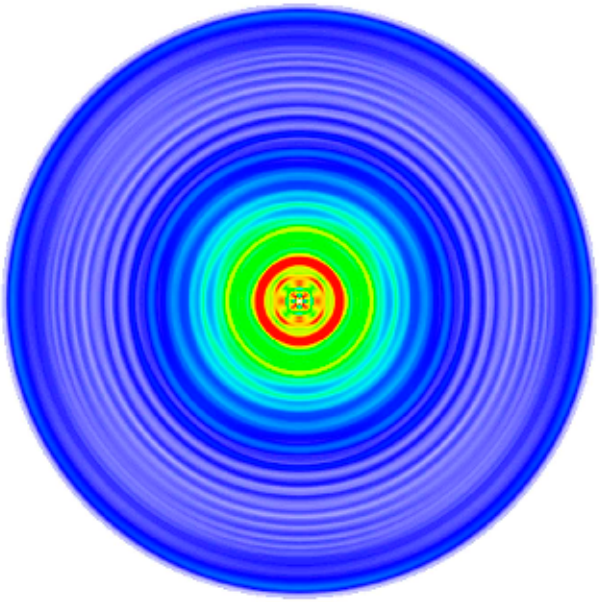

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Global potential energy surface of H_4^+ system. Reactive collisions using QCT

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H_4^+ is an important molecule in astrophysics because together with its isotopologues are involved in reactions of formation of H_3^+, the most abundant ion in space. We have calculated the first global potential energy surface for the ground electronic state of H_4^+ based on ab initio calculations. All studies of this system in the literature have made use of a DIM potential. The reaction of $H_2 + H_2^+ \rightarrow H_3^+ + H$ is an exothermic reaction with an energy of -1.81eV. The equilibrium geometry of H_4^+ can be seen as an isosceles H_3^+ with the fourth proton bound to the vertex created with the two elongated distances. The energy of the H_4^+ is its equilibrium is about 2eV below the entrance channel , $H_2 + H_2^+$. In addition, H_4^+ system presents a crossing between the ground and the first excited state in the entrance channel due to the equally probable position of the charge in either diatomic molecule. The crossing is produced when both molecules have the same interatomic distance. The lowest crossing in energy is obtained just above the first excited vibrational state of H_2 and the second excited vibrational state of H_2^+. The study of dynamics considering reactants in higher vibrational excited states than the ground state needs to treat this crossing to properly describe the position of the charge. In the literature the most common method describing the entrance channel is surface hoping.

In this contribution I will show as well the preliminary results obtained for the reactive collisions of $H_2 + H_2^+$ using quasiclassical trajectories. Results have been compared with other theoretical studies, which used the DIM potential approach, and with the available experimental studies in literature.